Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Spectroscopic and Second-order Nonlinear Optical Properties of Ruthenium(II) Complexes: A DFT/MRCI and ADC(2) Study

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Table S1. Excited-state composition of the FDAES of complex 4 at the ADC(2) and ADC(2)/COSMO levels.

ADC(2)

State	ΔE (eV)	f	Assignment (coeff.)
S_1	2.99	1.68	H→L $\pi\pi^*$ (0.83)

ADC(2)/COSMO

State	ΔE (eV)	f	Assignment (coeff.)
S_1	2.12	0.29	H-1→L MLCT (0.69)
			H→L $\pi\pi^*$ (0.41)
			H-1→L+1 MLCT (-0.41)

Table S2. Basis set dependence of selected electronic transition energies (in eV) and oscillator strengths (in parentheses) of complex 1 and 2 at the DFT/MRCI and ADC(2) levels of theory.

Complex	State	DFT/MRCI/ def2-SVP	DFT/MRCI/ def2-TZVP	ADC(2)/ def2-SVP	ADC(2)/ def2-TZVP
1	FDAES	2.80 (0.297)	2.86 (0.296)	3.03 (0.12)	2.72 (0.10)
2	FDAES	2.80 (0.537)	2.82 (0.545)	3.11 (0.23)	2.80 (0.19)

Figure S1. Main BH-LYP orbitals involved in the FDAES of complex 3 and 4.